

ELECTRON CAPTURE BY IONS PASSING THROUGH GASES

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ABSTRACT--The cross section for the capture in different excited s -states of an electron by an ion passing through gaseous matter has been evaluated ; the method followed is an extension to that of Brinkman and Kramers. It is found that the first term of the series obtained here for the $1s-n s$ capture agrees with Brinkman and Kramers' approximate result.

I N T R O D U C T I O N

The importance of the problem of the capture of an electron by an ion passing through gaseous matter has, of late, increased in view of its application to the explanation of some of the lines emitted by solar corona (Saha, 1942) and aurora borealis (Fan and Meinel, 1953). The theoretical study in this line has been mainly done by Oppenheimer (1928), Brinkman and Kramers (1930), Massey and Smith (1933), Saha and Basu (1945), Jackson and Schiff (1953) and others. Brinkman and Kramers have considered in detail the case in which an ion captures in its $1s$ orbit an electron which was originally in the $1s$ orbit of the atom constituting the gaseous matter. The present work is an extension of the theoretical investigation of Brinkman and Kramers for the more general case of capture of the electron in excited orbits. The necessity of considering the cross section of capture of electrons to excited orbits arises from the suggestion of Saha (1942) to explain the origin of He-lines in the spectrum of the chromosphere. In it we notice, in addition to the extremely strong neutral helium lines, the well-known line of ionised helium λ 4686Å whose appearance is unexpected in view of the fact that this line has an excitation potential of nearly 75.25 volts while the ordinary excitation of the chromosphere is 9 to 14 volts. The occurrence of this latter line has been explained by assuming that high velocity α -particles generated in the solar body due to some nuclear process get slowed down by losing energy through ionisation. After being considerably slowed down they begin to capture electrons in excited orbits which jump back to lower orbits emitting the well-known lines of ionised helium. The capture problem is expected to play an important role in explaining the spectrum of aurora borealis. The aurora borealis is most likely to be excited by high-speed ions penetrating into the upper atmosphere. Meinel (1951) detected a violet Doppler wing on

H α line extending to an energy greater than 57 Kev thus proving the existence of protons as one of those causing the excitation. A preliminary experiment by Meinel and Fan (1952) using accelerated protons with rarefied air sample, showed a striking similarity between the laboratory spectrum and that of the aurora.

DERIVATION OF THE RESULT

The type of collision considered in this paper comes under the general head of rearrangement collisions because here the electron initially attached to one hydrogen-like atom of charge Ze forms finally another hydrogen-like atom of charge $Z'e$ by simple rearrangement. The differential cross section of a general binary collision, in which a system A in state m collides with a system B in state n to form systems C in state s and D in state t , has been derived (Schiff, 1949) using the first Born approximation. In our problem, of the two initial systems, one is a hydrogen-like atom with charge Ze and mass AM of the nucleus to which an electron of charge $-e$ and mass m is bound in the n, l, m orbit and the other is a free particle with charge $Z'e$ and mass $A'M$ moving with the velocity \mathbf{v} with respect to the atom; the final systems are respectively a hydrogen-like atom with charge $Z'e$ and mass $A'M$ of the nucleus, the electron being in the n', l', m' orbit, and a free particle with charge Ze and mass AM relative to which the atom moves with a velocity \mathbf{v}' . Figure 1 gives us the co-ordinate system for our collision process.

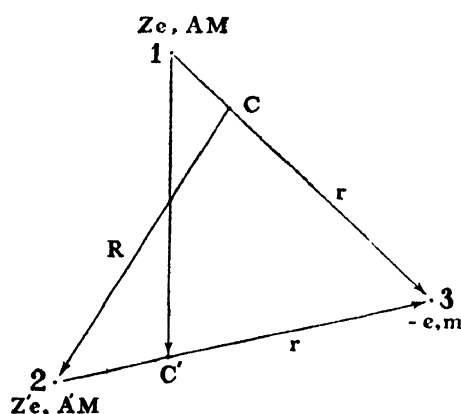


Figure 1. Co-ordinate system. The points marked C and C' are centres of mass of the initial and final atoms.

Following the calculations given in L. I. Schiff's 'Quantum Mechanics', we get the differential cross section for capture of the electron in the final n, l', m' state from the initial n, l, m state as in Jackson and, Schiff's paper (1953) viz,

$$\frac{dQ}{d\Omega} = \left(\frac{\mu f}{2\pi\hbar^2} \right) \left(\frac{v'}{v} \right) |I|^2, \quad (1)$$

$$\text{with } I = \int \exp(-i\mathbf{K}'\cdot\mathbf{R}') \psi_{n',l',m'}^*(\mathbf{r}') V \exp(i\mathbf{K}\cdot\mathbf{R}) \psi_{n,l,m}(\mathbf{r}) d\tau_r d\tau_{R'}, \quad (2)$$

where $\psi_{n,l,m}(\mathbf{r})$ is the normalised initial state wave-function for the electron in atom Z and $\psi_{n',l',m'}^*(\mathbf{r}')$ is the normalised final state wave function for the electron in the atom Z' ,

$$\left. \begin{aligned} (h/2\pi)\mathbf{K} &= \mu_i \mathbf{v} \\ (h/2\pi)\mathbf{K}' &= \mu_f \mathbf{v}' \end{aligned} \right\}, \quad (3) \quad \left. \begin{aligned} \mu_i &= A'M(AM+m)/(A+A')M+m \\ \mu_f &= AM(A'M+m)/(A+A')M+m \end{aligned} \right\}, \quad (4)$$

and V is the perturbation Hamiltonian.

Using as the independent coordinates \mathbf{r}, \mathbf{r}' instead of \mathbf{r}, \mathbf{R} we may write

$$I = \int \exp(-i\mathbf{C}\cdot\mathbf{r}') \psi_{n',l',m'}^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \exp(i\mathbf{B}\cdot\mathbf{r}) \psi_{n,l,m}(\mathbf{r}) d\tau_r d\tau_{r'}, \quad (5)$$

$$\text{where } \mathbf{C} = \mathbf{K} - \frac{A'M}{A'M+m} \mathbf{K}' \text{ and } \mathbf{B} = \frac{AM}{AM+m} \mathbf{K} - \mathbf{K}'. \quad (6)$$

The perturbation Hamiltonian consists of two parts ; (1) the Coulomb interaction between the electron and the incident particle and (2) the Coulomb interaction between the nucleus and the incident particle. Brinkman and Kramers (1930) considered only the first term neglecting the second one in their calculation of capture cross section for electrons from initial $1s$ orbit to final $1s$ orbit. Saha and Basu (1945) extended the method of Brinkman and Kramers to calculate the capture of electron from $1s$ to $2p$ orbit. It has been mentioned by Jackson and Schiff (1953) that in an exact calculation, the second term in the perturbation Hamiltonian would have actually a negligible contribution ; however, they claim that better results are obtained by taking into consideration the contribution of the second term which is no longer negligible when the calculations are based on the approximate method of Born. Here we shall follow Brinkman and Kramers, and shall carry out the calculation for the capture of electron in the final ns state from initial $1s$ state by the first of the two alternative methods given by them.

As the perturbation potential we may take either the initial perturbation

$$V_i = -\frac{Z'e^2}{r'} \text{ or the final perturbation } V_f = -\frac{Ze^2}{r}. \text{ However, it has been proved}$$

by Jackson and Schiff (1953) that in the first Born approximation the ambiguity in the choice of the perturbation potential does not lead to any ambiguity in the result for the transition probability. They show that when $V = V_i$

$$I = - \left(\frac{(h/2\pi)^2 C^2}{2m_f} + \epsilon_f \right) \phi_{n,l,m}(\mathbf{B}) \phi_{n',l',m'}^*(\mathbf{C}), \quad (7a)$$

and for $V = V_f$

$$I' = - \left(\frac{(h/2\pi)^2 B^2}{2m_i} + \epsilon_i \right) \phi_{n,l,m}(\mathbf{B}) \phi_{n',l',m'}^*(\mathbf{C}), \quad (7b)$$

where m_i and m_f are the reduced masses of the electron when attached to the atoms Z and Z' respectively

$$m_i = \frac{AMm}{AM+m} \text{ and } m_f = \frac{A'Mm}{A'M+m}, \quad (8)$$

$$\phi_{n,l,m}(\mathbf{B}) = \int \exp(i\mathbf{B} \cdot \mathbf{r}) \psi_{n,l,m}(\mathbf{r}) d\tau_r \quad (9)$$

$$\phi'_{n',l',m'}(\mathbf{C}) = \int \exp(i\mathbf{C} \cdot \mathbf{r}') \psi'_{n',l',m'}(\mathbf{r}') d\tau_{r'}$$

and ϵ, ϵ' are the binding energies of the electron in atoms Z and Z' respectively.

Now from the conservation of energy requirement viz.,

$$\frac{1}{2} \mu_i v^2 - \epsilon - \frac{1}{2} \mu_f v'^2 - \epsilon',$$

we get with the help of equations (4), (6) and (8)

$$\frac{(h/2\pi)^2 C^2}{2m_f} + \epsilon' = \frac{h^2 B^2}{2m_i} + \epsilon \quad (10)$$

Hence $I = I'$.

The evaluation of $\phi_{n,l,m}(\mathbf{K})$ for a hydrogen-like atom with charge Ze of the nucleus has been done by Podolsky and Pauling (1929):

$$\phi_{n,l,m}(\mathbf{K}) = \left\{ \frac{1}{(2\pi)^{1/2}} e^{im\beta} \left\{ \left(\frac{(2l+1)(l-m)!}{2(l+m)!} \right)^{1/2} P_l^m(\cos\alpha) \right\} \right. \\ \left. - \frac{(i)^l \pi 2^{2l+4} l!}{\gamma_n^{1/2}} \left(\frac{n(n-l-1)!}{(n+l)!} \right)^{-1} \frac{\zeta^{l+1}}{(\zeta^2+1)^{l+1/2}} C_{n-l-1}^{l+1} \left(\frac{\zeta^2-1}{\zeta^2+1} \right) \right\}, \quad (11)$$

where K, α, β are the polar co-ordinates of \mathbf{K} ,

$$\zeta = \frac{K}{\gamma_n} \text{ with } \gamma_n = \frac{Z}{na} = \frac{Ze^2 m^*}{n\hbar^2}, \text{ } m^* \text{ being the reduced mass of the electron in}$$

the atom, and C_q'' is the Gegenbauer function which may be defined by the generating function

$$Q \equiv (1-2ut+u^2)^{-n} = \sum_{q=0}^{\infty} C_q''(t) u^q, \quad (12)$$

$$u < 1$$

Hence from (1), (7) and (11), the differential cross section is known in general for capture of the electron in any final state from any initial state.

From (11) we have in particular

$$\phi_{1,0}(\mathbf{B}) = -8\pi^{1/2} \gamma_1^{5/2} (B^2 + \gamma_1^2)^{-2} \\ \phi_{n,0}(\mathbf{C}) = -8\pi^{1/2} \gamma_n^{5/2} (C^2 + \gamma_n^2)^{-2} C_{n-1}^1 \left(\frac{C^2 - \gamma_n^2}{C^2 + \gamma_n^2} \right), \quad (13)$$

$$\text{where } \gamma_1 = \frac{Z}{a_0} \quad \text{with} \quad a_0 = \frac{\hbar^2}{m_i e^2} \quad (14)$$

$$\text{and } \gamma'_n = \frac{Z'}{na'_0} \quad \text{with} \quad a'_0 = \frac{\hbar^2}{m_f c^2} \quad \left| \right.$$

With the help of (7) and (10) we get

$$I = 2\pi \hbar^2 \frac{m_f}{m_i^2} \gamma_1^{5/2} \gamma'_n{}^{5/2} (C^2 + \gamma'_n{}^2)^{-3} C^{n-1} \left(\frac{C^2 - \gamma'_n{}^2}{C^2 + \gamma'_n{}^2} \right) \quad (15)$$

To get the total cross section we require the integral of $|I|^2$ over all directions of orientation of the solid angle Ω . Now $C^{n-1}(\cos \Theta)$ is the coefficient of u^{n-1} in the expansion of $(1 - 2u \cos \Theta + u^2)^{-1}$ when $u < 1$. (cf. eqn. (12)).

Hence

$$\{C^{n-1}(\cos \Theta)\}^2 = \left\{ \frac{\sin n\Theta}{\sin \Theta} \right\}^2 = 2 \sum_{r=0}^{n-1} (-)^r \frac{n^2(n^2-1^2)\dots(n^2-r^2)}{\{2(r+1)\}!} (2 \sin \Theta)^2 \quad (16)$$

Putting

$$\frac{C^2 - \gamma'_n{}^2}{C^2 + \gamma'_n{}^2} = \cos \Theta = 1 - 2x, \quad (17)$$

we have

$$1 - \frac{\gamma'_n{}^2}{C^2 + \gamma'_n{}^2} = \frac{1 - \cos \Theta}{2} \quad (18)$$

$$x(1-x) = \frac{(\gamma'_n{}^2)^2}{(C^2 + \gamma'_n{}^2)^2} = \frac{1}{4} \sin^2 \Theta, \quad (19)$$

and from (6)

$$d\lambda = -2\lambda K K' \frac{\gamma'_n}{(C^2 + \gamma'_n{}^2)^2} \sin \theta d\theta, \quad (20)$$

where $\lambda = A'M/(AM+m)$ and θ is the angle between \mathbf{K} and \mathbf{K}' . Thus utilising the above results we get from (15),

$$2\pi \int_0^\pi |I|^2 \sin \theta d\theta = \frac{2^{10}\pi^3 \hbar^4 m^2 r \gamma_1^{5/2}}{\lambda K K' m^4 i \gamma'_n{}^{5/2}} \sum_{r=0}^{n-1} \int_{x(\theta=\pi)}^{x(\theta=0)} \frac{S_r(O,n) x^{1+r}}{x(\theta=\pi)} (1-x)^r dx, \quad (21)$$

$$\text{with} \quad S_r(O,n) = (-)^r 2 \frac{n^2(n^2-1^2)\dots(n^2-r^2)}{\{2(r+1)\}!} 4^{2r}. \quad (22)$$

Under the usual condition

$$\begin{aligned} K &\simeq \lambda K' \gg \gamma'_n \\ &\gg |K - \lambda K'| \end{aligned} \quad (23)$$

Then from (18) and (6) we have

$$x(\theta=\pi) = \frac{\gamma' n^2}{(K + \lambda K')^2 + \gamma' n^2} \approx 0$$

and

$$x(\theta=0) = x_0 = \frac{\gamma' n^2}{(K - \lambda K')^2 + \gamma' n^2} \approx \gamma' n^2 / \left\{ \frac{1}{2} (\gamma_1^2 + \gamma'^2) + \pi^2 \sigma^2 + \frac{(\gamma_1^2 - \gamma' n^2)^2}{16\pi^2 \sigma^2} \right\}, \quad (\text{vide appendix}) \quad (24)$$

with

$$\sigma = \frac{mv}{h}.$$

For the evaluation of the integral in the right hand side of the eqn. (21), we may note that $\int_0^{x_0} x^{4+r} (1-x)^r dx$ is the incomplete beta-function $B_{x_0}^1(5+r, 1+r)$ the numerical value of which can be obtained easily.

Now since $m \ll M$ we may write $\mu_f \approx \mu_i$, $m_f \approx m_i \approx m$, $\lambda \approx 1$, and $a'_0 \approx a_0$. Hence from (1) & (21) the total capture cross section from 1s orbit to ns orbit is given by

$$Q = 2^8 \pi \frac{e^4}{(h^2/2\pi)^2 v^2 a_0^2} \left(\frac{nZ}{Z'} \right)^2 \sum_{r=1}^{n-1} S_r(O, n) B_{x_0}(5+r, 1+r). \quad \dots \quad (25)$$

DISCUSSION

The expression given by B. K. for the 1s-ns capture cross section is approximate being only the first term of our series in eqn. (25). In fact the contribution of the other terms of the series is not at all negligible for low energy of the incident particle. However, for very high energy of the incident particle the result on the basis of our expression differs very little from that of B. K., the main contribution being due to the first term. Thus at high energies of the incident particle we have an inverse n^3 law for the capture cross section as given also by Oppenheimer.

APPENDIX

To prove

$$\gamma' n^2 + (K - \lambda K')^2 \approx \frac{1}{2} (\gamma_1^2 + \gamma' n^2) + \pi^2 \sigma^2 + \frac{(\gamma_1^2 - \gamma' n^2)^2}{16\pi^2 \sigma^2},$$

we have from (3) and (4)

$$(K - \lambda K')^2 = \frac{4\pi^2}{S^2} \left\{ \frac{AM \cdot A'M}{h} (v - v') + A'M\sigma \right\}^2$$

where

$$S = (A + A')M + m$$

and

$$h = mv$$

From (10) we may write with the help of (3), (4), (6) and (14),

$$\begin{aligned} & \gamma'^2 + \frac{4\pi^2}{S^2} \left\{ \frac{AM.A'M}{h} (v-v') + A'M\sigma \right\}^2 \\ &= \gamma_1^2 + \frac{4\pi^2}{S^2} \left\{ \frac{AM.A'M}{h} (v-v') - AM \cdot \frac{mv}{h} \right\}^2 \\ &\simeq \gamma_1^2 + \frac{4\pi^2}{S^2} \left[\left\{ \frac{AM.A'M}{h} (v-v') + A'M\sigma \right\} - S\sigma \right]^2 \end{aligned}$$

upto the first order of approximation. We take $(v-v')/v$ and m/M as small quantities of the first order.

Then

$$\frac{2\pi}{S} \left\{ \frac{AM.A'M}{h} (v-v') + A'M\sigma \right\} = \frac{\gamma_1^2 - \gamma'^2}{4\pi\sigma} + \pi\sigma.$$

Hence follows the result.

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